SURFACE CONDUCTIVITY AS A NATURAL PROPERTY FOR HYDROGENATED DIAMOND

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Abstract

The electronic structure with Milliken occupation of a series of diamond clusters with hydrogen-terminated surface has been calculated by means of density functional theory (DFT). From the obtained results it is found that the Fermi-level (E_F) of clusters lowers with the clusters-size increasing. Combining this finding with the localization character of states in the noncrystalline surface layer, we may conclude that (1) every crystalline particle is composed geometrically of two phases, one is of the surface noncrystalline layer in which the E_F is lower than that of the whole cluster and the electrons are trapped in localized states; another phase is the interior crystal in which the electron is quasi-free in delocalized states similar to that in bulk metal; (2) existence of the layer with trapped-electron at surface and free-hole-accumulation inside and near surface is the origin of surface conductivity in diamond and various impurities as well as defects at surface play the role of changing the electron distribution in the surface region, namely, they do not originally affect the surface conductivity.

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